

SAFETY DATA SHEET according

to GB/T 16483 and GB/T 17519

Version 6.1 Revision Date 06.03.2021 Print Date 27.04.2023 Date of first issue 20.06.2018

SDS No. Aldrich - 58825 Product Number Aldrich - 58825

tert-Butyl isocyanoacetate

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : tert-Butyl isocyanoacetate

Product Number : 58825 Brand : Aldrich CAS-No. : 2769-72-4

1.2 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich (Shanghai) Trading Co.Ltd.

509 Renging Road

Zhangjiang High Tech East Park, Pudong

SHANGHAI

201201 SHANGHAI

CHINA

西格玛奥德里奇(上海)贸易有限公司 **上海市浦**东新区仁庆路 509 号 10 幢

邮政编码: 201201

Telephone : +86 21 6141-5566 Fax : +86 21 6141-5567

1.3 Emergency telephone

Emergency Phone # : +86 532 83889090

1.4 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : For R&D use only. Not for pharmaceutical, household or other

uses

SECTION 2: Hazards identification

Summary of emergency

clear, liquid dark brown Combustible liquid., Harmful if swallowed or if inhaled. Consult a physician., Show this material safety data sheet to the doctor in attendance. If breathed in, move person into fresh air., If not breathing, give artificial respiration., Consult a physician. Wash off with soap and plenty of water., Consult a physician. Flush eyes with water as a precaution. Do NOT induce vomiting., Never give anything by mouth to an unconscious person., Rinse mouth with water., Consult a physician.

Aldrich- 58825 Page 1 of 9



2.1 GHS Classification

Flammable liquids (Category 4), H227 Acute toxicity, Oral (Category 4), H302 Acute toxicity, Inhalation (Category 4), H332

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning

Hazard statement(s)

H227 Combustible liquid.

H302 + H332 Harmful if swallowed or if inhaled.

Precautionary statement(s)

Prevention

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No

smoking.

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

P280 Wear protective gloves/ eye protection/ face protection.

Response

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel

unwell. Rinse mouth.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable

for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant

foam to extinguish.

Storage

P403 + P235 Store in a well-ventilated place. Keep cool.

Disposal

P501 Dispose of contents/ container to an approved waste disposal

plant.

Caution - substance not yet tested completely.

Reduced Labeling (<= 125 ml)

Pictogram

Signal word Warning

Hazard statement(s)

H227 Combustible liquid.

H302 + H332 Harmful if swallowed or if inhaled.

Precautionary none

statement(s)

2.3 Physical and chemical hazards

H227 Combustible liquid.

2.4 Health hazards

H302 Harmful if swallowed. H332 Harmful if inhaled.

2.5 Environmental hazards

Referring to current information, no environmental hazard.

2.6 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Formula : $C_7H_{11}NO_2$ Molecular weight : 141.17 g/mol CAS-No. : 2769-72-4

Hazardous ingredients

Component	Classification	Concentration
tert-Butyl isocyanoacetate		
	Flammable liquids Category 4; Acute toxicity Category 4; H227, H302, H332	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

Merck

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NOx)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary. Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place.

Storage stability

Aldrich- 58825 Page 4 of 9

Light sensitive. Store under inert gas.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

0.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid

Color: dark brown

b) Odorc) Odor Thresholdd) pHNo data availableNo data available

Aldrich- 58825 Page 5 of 9



e) Melting No data available point/freezing point Initial boiling point 50 °C at 0.1 hPa and boiling range g) Flash point 82 °C - closed cup No data available h) Evaporation rate Flammability (solid, No data available i) gas) No data available Upper/lower j) flammability or explosive limits k) Vapor pressure No data available Vapor density No data available m) Relative density No data available n) Water solubility insoluble o) Partition coefficient: No data available n-octanol/water p) Autoignition No data available

temperature q) Decomposition

temperature

No data available

Viscosity Viscosity, kinematic: No data available r) Viscosity, dynamic: No data available

No data available s) Explosive properties Oxidizing properties No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

Stable under recommended storage conditions.

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

Heat, flames and sparks.

10.4 Incompatible materials

Oxidizing agents

10.5 Hazardous decomposition products

In the event of fire: see section 5

MGBCK

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

No data available LD50 Oral - 500.1 mg/kg LC50 Inhalation - 4 h - 11 mg/l (Acute toxicity estimate)

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No ingredient of this product present at levels greater than or equal to 0.1% is

identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

Aldrich- 58825

No data available



Page 7 of 9

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2810 IMDG: 2810 IATA-DGR: 2810

14.2 UN proper shipping name

ADR/RID: TOXIC LIQUID, ORGANIC, N.O.S. (tert-Butyl isocyanoacetate) IMDG: TOXIC LIQUID, ORGANIC, N.O.S. (tert-Butyl isocyanoacetate) IATA-DGR: Toxic liquid, organic, n.o.s. (tert-Butyl isocyanoacetate)

14.3 Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA-DGR: 6.1

14.4 Packaging group

ADR/RID: III IMDG: III IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport. Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

Oxidizing agents

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

MERCK

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H227 Combustible liquid. H302 Harmful if swallowed. H332 Harmful if inhaled.

Further information

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Aldrich- 58825 Page 9 of 9

